Unstructured Mesh Overview

Technical Leads

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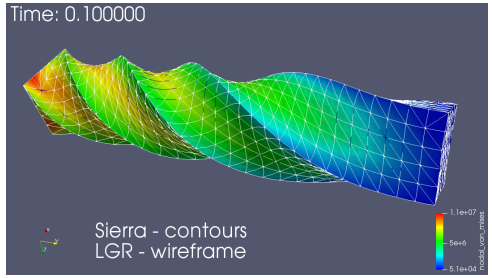
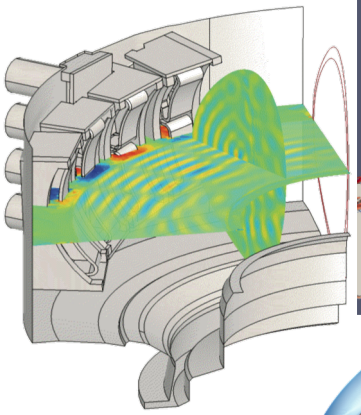
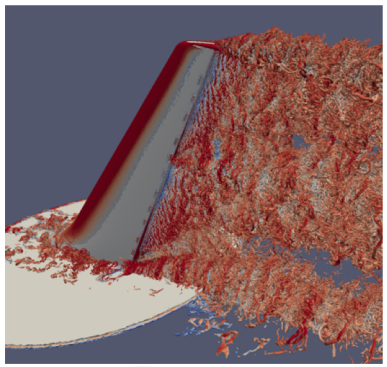
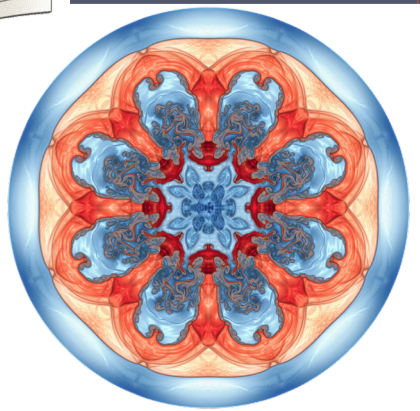
Unstructured Mesh Analysis Codes

- FASTMath Activities
  - Develop unstructured mesh-based analysis tools
  - Demonstrate performance at full machine scale
  - Consider alternative equation discretization methods
  - Apply these analysis technologies towards applications
- Relevant Software Tools
  - MFEM – High Order F.E. Library
  - Albany/LGR – PDE solution application, large deformation mechanics
  - PHASTA – Navier-Stokes flow solver
- Applications Impacted
  - Fusion
  - Non-linear large deformation solid mechanics
  - Shock hydrodynamics
  - CFD applications









Our unstructured mesh tools are used in many apps: from elasticity, to incompressible and compressible flows, and fusion

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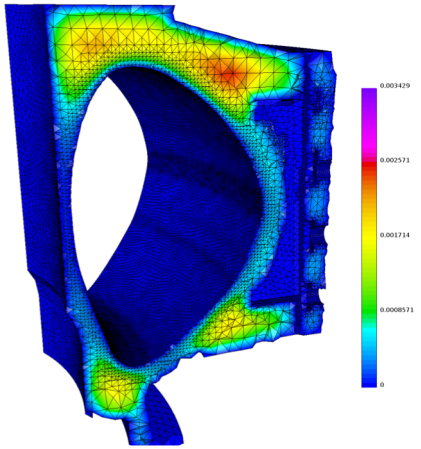
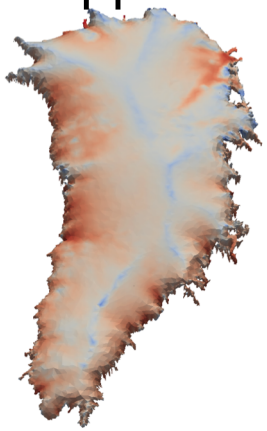
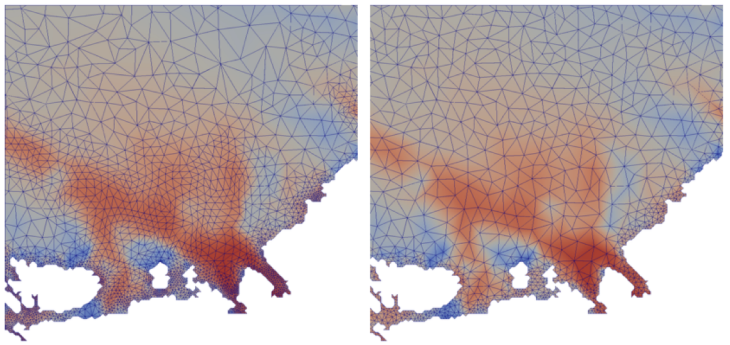
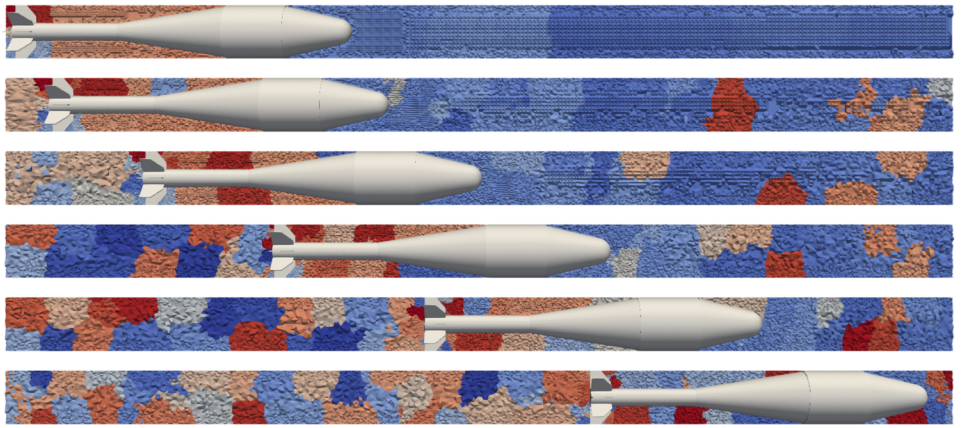
Unstructured Mesh Adaptation Technology

- FASTMath Activities
  - Provide parallel unstructured mesh adaptation technologies for both low order and high-order methods
  - Conforming and non-conforming adaptation
  - Integrate these technologies with applications
- Relevant Software
  - Omega_h
  - MFEM
  - PUMI
  - MeshAdapt
- Applications Impacted
  - Albany/LGR for non-linear large deformation solid mechanics
  - M3D-C1, GITR, hPIC and XGC for Fusion for PIC codes
  - MFEM for Fusion, Flow, Elasticity and High-Order applications
  - PHASTA for CFD applications









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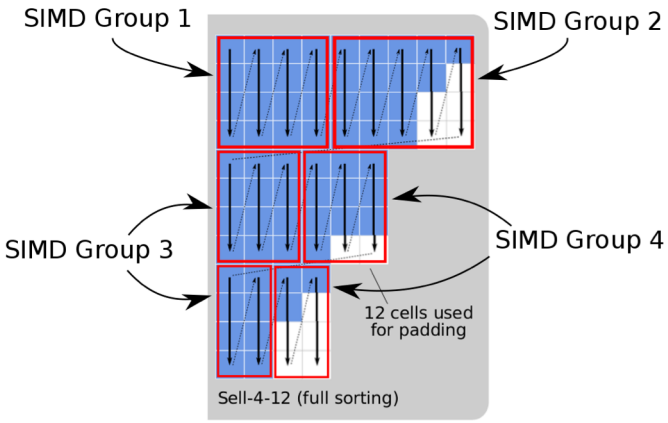
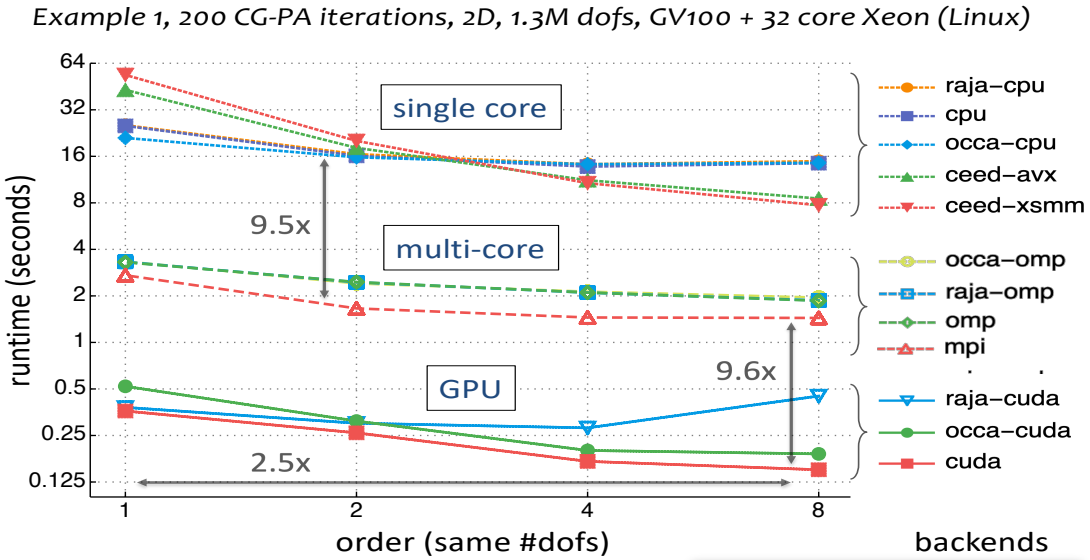
Performant Unstructured Meshes



SCS for particles on mesh

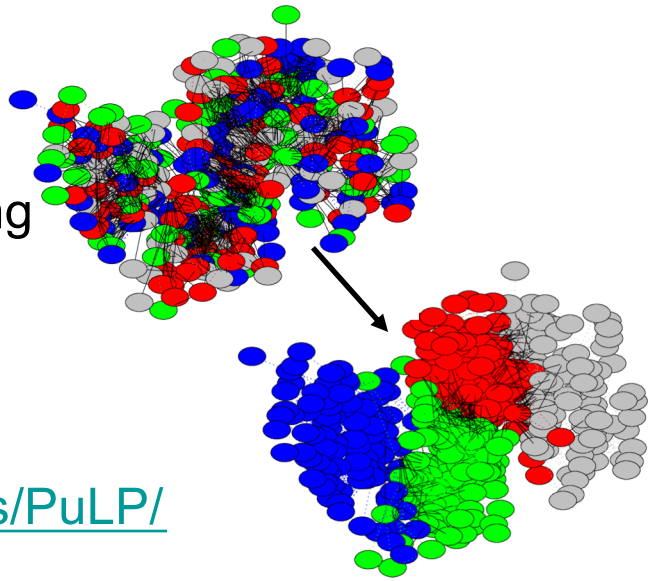
- FASTMath Activities
  - Develop unstructured meshing technologies that execute on near exascale systems
  - Support interactions between solvers and unstructured meshes
  - Integrate these technologies into unstructured mesh simulation tools
- Relevant Software Tools
  - Omega_h, MFEM, PHASTA, EnGPar, PUMIpic
- Applications Impacted
  - XGC, GITR & M3D-C[1]Fusion
  - MFEM for Fusion and other applications
  - PHASTA for CFD applications
  - Albany/LGR Non-linear large deformation solid mechanics



Initial results with MFEM v4.0

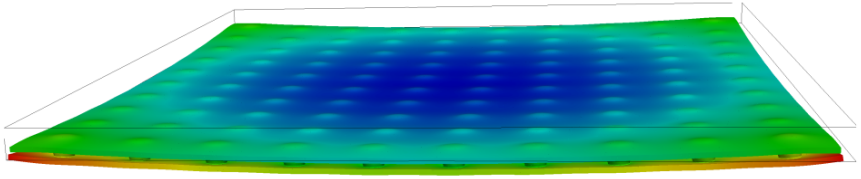
FASTMath provides advanced dynamic load balancing and task mapping for extreme scale applications

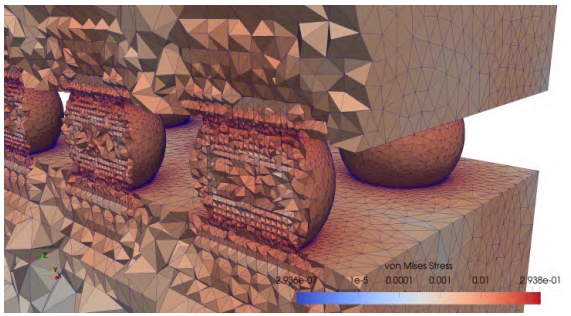
- **FASTMath Activities**
  - Massively parallel graph algorithms
  - Architecture aware load balancing and task mapping
  - Multi-criteria dynamic partition improvement
- **Relevant Software Tools**
  - PuLP and XtraPuLP: Graph Partitioning using Label Propagation - github.com/HPCGraphAnalysis/PuLP/
  - Zoltan and Zoltan2 - www.cs.sandia.gov/zoltan/
  - EnGPar – scorec.github.io/EnGPar/
- **Applications Impacted**
  - Albany Multiphysics
  - XGC, GITR – fusion
  - MFEM
  - E3SM HOMME
  - NNSA Sierra



The XtraPuLP graph partitioner can compute balanced multi-object partitionings of irregular trillion-edge graphs in minutes

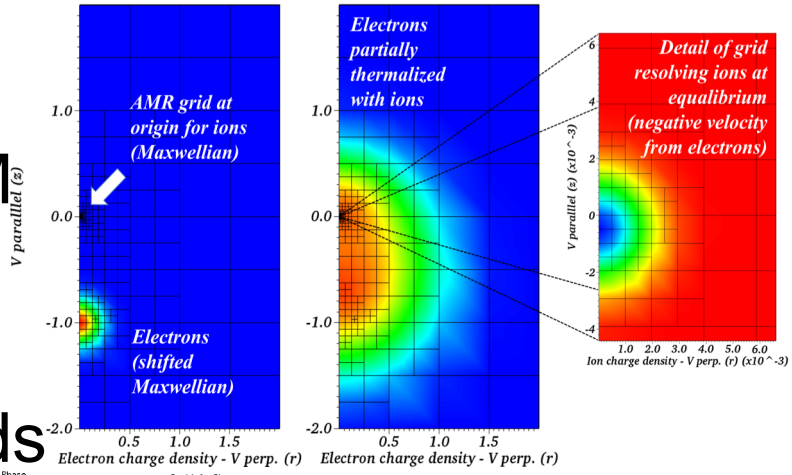
Error-driven in-memory mesh adaptation of thermal creep in a flip-chip using Albany Multiphysics and Zoltan

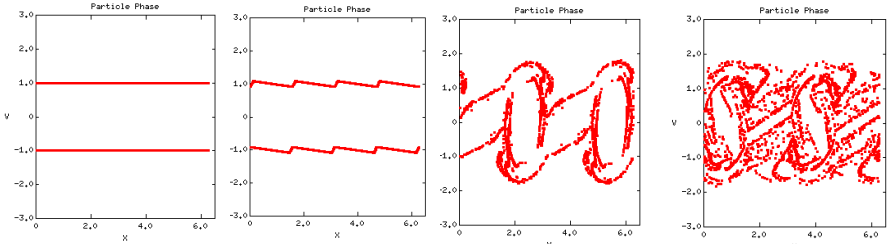




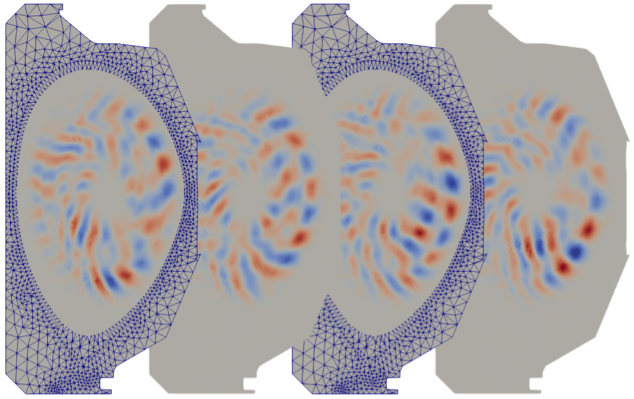
Unstructured Mesh Methods for Particle in Cell Simulations

- FASTMath Activities
  - Conservative coupled particle/FEM method for the Vlassov-Maxwell-Laundau system
  - Parallel unstructured mesh methods for PIC simulation codes
- Applications Impacted
  - Fusion Edge Plasma – XGC
  - Fusion impurity modeling – GITR
  - Core Plasma – GEMPIC, M3D-C1pic





Two stream instability test, initial conditions (left), with roll up (right) using initial PETSc implementation of GEMPIC



Snapshot of electrostatic potential fluctuation at toroidal angle $\zeta=0,\pi/2,\pi,3\pi/2$ from left to right for mesh-based XGC

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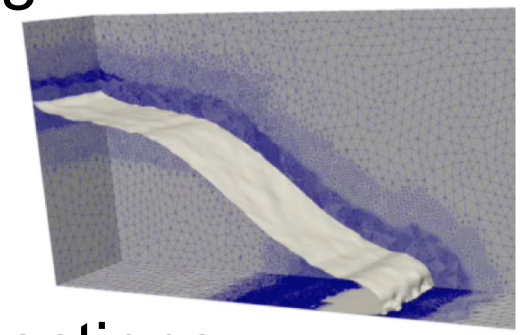
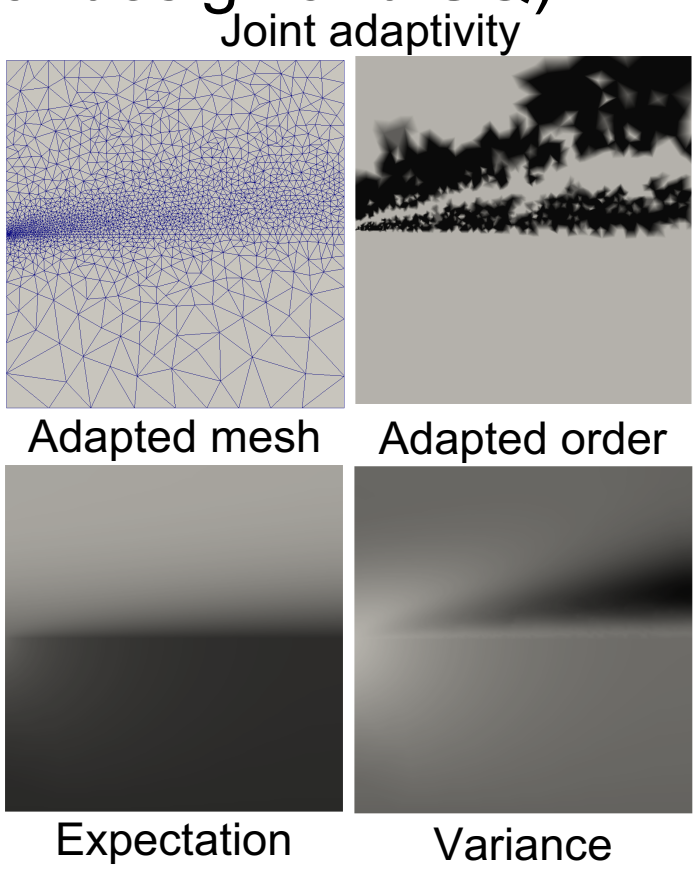
Data Analytics for Unstructured Meshes

- Extraction of reliable engineering predictions and fundamental insights from simulations becomes challenging when:
  - Geometry is complex and evolving (e.g., physics-driven)
  - Discretization is large (even with adaptivity)
  - Number of input parameters is high (for design and UQ)
- FASTMath Activities
  - Unstructured mesh management
  - Computational steering
  - Multi-fidelity modeling
  - In situ visualization
- Applications Impacted
  - Flow applications
  - Plasma surface interactions





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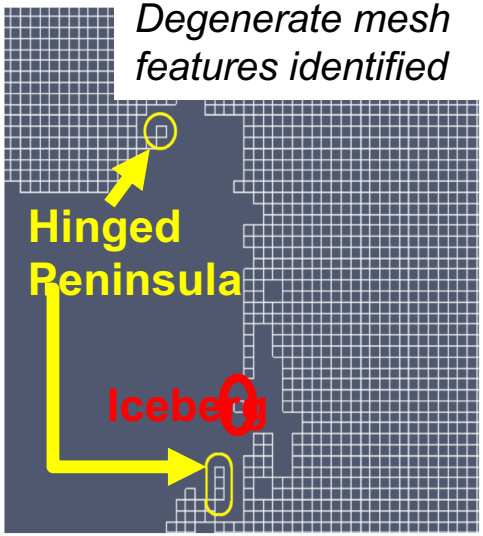
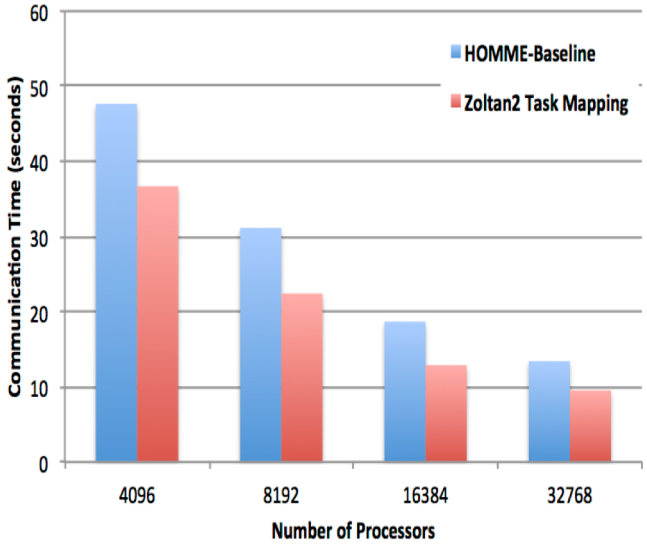
SciDAC ProSPecT, E3SM and Zoltan2: Graph Algorithms, Task Mapping, and Partitioning

- Graph Algorithms for SciDAC ProSPect Ice Sheet Modeling
  - Algorithms developed to identification degererate mesh features
  - Zoltan2's biconnected-component algorithms reduce time for degenerate mesh feature detection
- HOMME: High-Order Method Modeling Environment for atmospheric modeling
  - Unstructured quadrilateral meshes on the sphere
  - Zoltan2's geometric task placement reduces HOMME's communication time
- Partitioning in E3SM Climate Component Coupler
  - Zoltan's multi-weight geometric partitioners spatially align meshes so that little communication is needed during search and transfer





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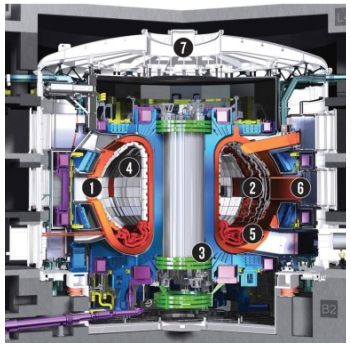
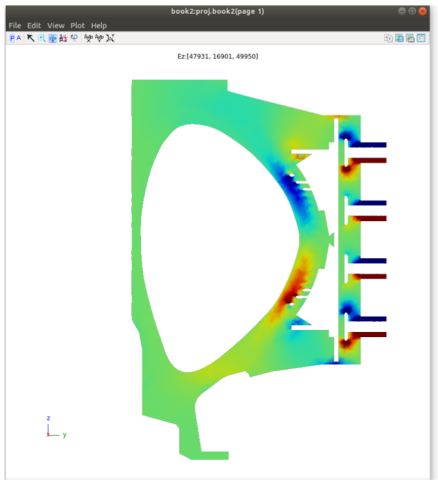
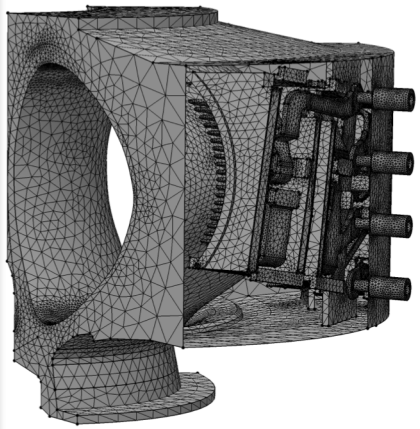
E3SM Energy Exascale Earth System Model

Fusion SciDAC Unstructured Mesh Needs

- Unstructured mesh technologies for four fusion SciDACs
  - Center for Tokamak Transient Simulations, Steve Jardin, PPPL
  - High-fidelity Boundary Plasma Simulation, C.S. Chang
  - Int. Simulation of Fusion Relevant RF Actuators, Paul Bonoli, MIT
  - Plasma Surface Interactions, Brian Wirth, ORNL
- Unstructured mesh capabilities being provided
  - Combined physical and physics model entities
  - CAD model simplification
  - Mesh generation with specific mesh controls
  - Adaptive simulation workflows
  - Analysis code mesh infrastructure including assembly
  - Parallel mesh based PIC methods for three PIC codes







MFEM Result z-component of electric field on a x-plane cut view (1M ele.)

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Unstructured Mesh Collaborations

- Within FASTMath
  - Solvers – Supporting mesh-based analysis codes
  - UQ – Unstructured meshes for UQ, UQ with adapted mesh
  - DATA – in situ data analytics
- With Rapids
  - In situ visualization and data methods
  - Performance of mesh adaptation
  - Methods to more effectively execute workflows
- With ECP (taking advantage of ECP developments)
  - CEED co-design center exascale discretizations
  - Fusion WDM application – coupling strategies
  - COPA co-design center for particle applications

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Summary of Posters:

- Unstructured Mesh Analysis Codes
- Unstructured Mesh Adaptation
- Performant Unstructured Mesh Technologies
- Dynamic Load Balancing and Task Mapping for Extreme-Scale Dynamic Applications
- Unstructured Mesh Methods for Particle in Cell Simulations
- Data Analytics for Unstructured Meshes
- SciDAC ProSPecT, E3SM and Zoltan2: Graph Algorithms, Task Mapping, and Partitioning
- Unstructured Mesh Technologies for the Fusion SciDAC Centers

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